CHLORANTHALACTONE A

66395-02-6 | DTXSID90318686

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 312 °C

Global applicability domain: Inside

Local applicability domain index: 4.29e-01

Confidence level: 6.54e-01

Nearest Neighbors from the Training Set

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Phosphine, ethyldiphenyl-

Measured: 293 Predicted: 310

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4-Bromobenzophenone

Measured: 350 Predicted: 336

Image not found

2-Propanone, 1,3-diphenyl-

Measured: 331 Predicted: 327

Image not found

4-Chlorobenzophenone

Measured: 332 Predicted: 320